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AN HP-97/67 PROGRAM FOR CALCULATION OF HYDROCARBON VAPOUR CONCENTRATIONS IN AIR

by

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ABSTRACTS

Calculations for gas detector calibration and other applications are automated with an HP-97/67 calculator program which solves for an unknown variable, given two others. The three variables are enclosure volume, hydrocarbon liquid volume and vapour concentration. A data card provides information for an initial group of some twenty different hydrocarbons.

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INTRODUCTION

During the course of combustible gas detection instrument evaluation and explosion testing with hydrocarbon vapours, a routine set of calculations must be performed which determine the amount of hydrocarbon liquid to be vapourized in an enclosed air atmosphere in order to attain a desired vapour concentration. This report describes a program for Hewlett-Packard Models 97 and 67 calculators which eliminates the associated manual calculations and reference searching for an initial group of twenty hydrocarbons.

Once the hydrocarbon of interest has been selected, three variables are available to the user - enclosure volume, desired vapour concentration and volume of hydrocarbon liquid. The program is designed to automatically calculate whatever third variable is left after the first two have been keyed in.

This program assumes ideal gas behaviour, binary mixtures, a temperature of 20°C during vapourization of the liquid, and a pressure of one atmosphere. As long as ideal gas behaviour is adhered to once the liquid has been vapourized however, the volumetric concentration of vapour remains the same at any given temperature and pressure. This also assumes that no condensation takes place. If any doubt as to non-ideality exists the reader is referred to Van der Waals' equation of state for real gases.

METHOD

Any ideal gas or vapour follows the relation

$$PV = nRT \quad \text{_____(1)}$$

where P = Pressure in atmospheres

V = Volume in litres

n = Number of moles of component of interest

R = Ideal gas constant = .08206

T = Temperature in ^{o}K.

If a chamber having volume V_c with vapour concentration X(in % by volume) will contain a vapour volume

$$V_v = \frac{V_c \, x}{100} \text{ litres} \quad \text{_____(2)}$$

the balance being air.

Sustituting (2) into (1) and rearranging yields

$$n = \frac{PV_c x}{100\ RT} \quad \text{_____(3)}$$

The relation between number of moles and volume of liquid required is given by

$$v = \frac{nW}{d} \quad \text{_____(4)}$$

where V = volume in millilitres

n = number of moles

W = moleculor weight of component of interest in grams per mole

d = density in grams per millilitre

Rearranging yields

$$v = \frac{PV_g \, Wx}{100\ dRT} \quad \text{_____(5)}$$

This equation is used by the calculator to determine the required liquid volume, or, by rearrangement, the other two unknowns (V_l and x).

USING THE PROGRAM

Because a considerable amount of data is stored in the program, both a data card and a program card must be passed through the card reader. Each data card contains information for up to twenty combustible vapours, and each vapour is assigned a reference number (see Table 1). For example, if it is desired to obtain data about methyl ethyl ketone, its reference number, 10, is keyed into the display. Button A is then pushed which causes the calculator to retrieve the appropriate information from memory preparatory to the next calculation.

Button B is pushed after the volume of the chamber (in cubic feet) has been keyed into the display. The calculator assumes units of cubic feet but if it is desired to work in litres, button b is first pushed (a 1 will appear), after which all chamber volumes must be entered in litres. Push b to revert to cubic feet again (a 0 will appear). If button B is pushed but no data has been entered, the calculator assumes that both the liquid volume and desired vapour concentration data have been entered, and will proceed to calculate the necessary chamber volume, which will be displayed in the selected units.

Button C is pushed after the hydrocarbon liquid volume (in millilitres) has been keyed into the display. If button C is pushed but no data has been entered, the calculator assumes that both chamber volume and desired vapour concentration data have been entered, and will proceed to calculate the necessary hydrocarbon liquid volume, which will be displayed in millilitres.

Either button D or E may be pushed to enter desired vapour concentration. Button D assumes that the keyed in data is expressed as a percentage of the lower flammable limit of the substance selected, and button E assumes that the keyed in data is expressed as a percentage of the total volume of the chamber. Vapour concentration as a result of calculations will be displayed in either % LFL or % of total chamber volume. This display mode is selected by pressing button E, and pressing again to revert to the alternate mode with % LFL being the initial display mode.

To obtain the lower flammable limit of the selected vapour, press button D, and it will be displayed in per cent by volume.

EXAMPLES

1. What volume of hexane liquid is required to obtain a 50% LFL concentration in a 5 cubic foot enclosure?

		Press
Load Program card		
Load data card		
Select hexane		8
		A
Key in chamber volume		5
		B
Key in desired % LFL		50
		D
Volume of liquid		C
Displayed answer:	4.615 ml	

2. How large an enclosure would be required to create a 2% by volume concentration of Methyl Ethyl Ketone if 5 ml of the liquid is available for vapourization? Display the answer in litres.

Select MEK		10
		A
Select litres for enclosure volume		b
Enter desired concentration		2
		E
Enter liquid volume		5
		C
Enclosure size:		B
Displayed answer:	67.1 litres	

3. The binary mixture apparatus of the Canadian Explosive Atmospheres Laboratory has a volume of 14.18 litres. What volume of cyclohexane liquid is required to generate a 50% LFL mixture?

Select Cyclohexane	0
	A
Enter desired concentration	50
	D
Enter enclosure size	14.18
	B
Liquid volume	C

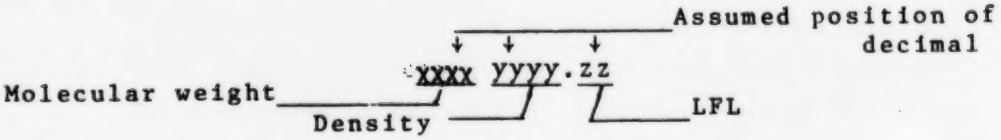
Answer: .414 ml

If relatively high concentrations of vapour are encountered, it would be wise to check that these concentrations are still below the saturated level. For some of the materials, no flammable limit has been stored on the data card due to a lack of available information at time of writing.

DATA CARD PREPARATION

The HP97/67 program, illustrated in Fig. 1, enables the user to select a given hdyrocarbon from the information which has been stored on the data card and loaded into the calculator. Additional data cards may be prepared by the user to accommodate information relating to substances of specific interest and not stored on data card No. 1. The following shows how this data card information is stored and assumes some knowledge of HP97/67 operations.

Each substance is assigned one memory location (from R_0 to R_{19}) which stores the following information: molecular weight, density and lower flammable limit. Registers R_I and R_A to R_E are not used to store data, but are used within the program for other purposes. For example, cyclohexane, which has a molecular weight of 84.2, a density of 0.779 g/ml. and an LFL of 1.3% by volume would have the number 08420779.13 stored in its memory register. The formatting is, therefore:



When retrieving this number from memory, the calculator will atuomatically place a decimal point between the first and second digits of molecular weight (counting from the right), between the third and fourth digits of density and between the first and second digits of LFL. It can be seen that this system accommodates molecular weights up to 999.9, densities up to 9.999 g/ml and LFL up to 9.9% by volume.

Another example is n-Octane, having a molecular weight of 114.2, density of 0.703 and LFL of 1.0% by volume. This information is stored as 11420703.10 in register R_{12} on data card No. 1, the contents of which are shown in Table 2.

TABLE 1

Reference Number	Material
0	Cyclohexane
1	2 - Propanone (Acetone)
2	Toluene
3	Ethanol (Ethyl Alcohol)
4	Methanol (Methyl Alcohol)
5	Ethyl Acetate
6	di-Ethyl Ether
7	n-Heptane
8	Hexane
9	2 - Propanol (Isopropyl Alcohol)
10	MEK (Methyl Ethyl Ketone)
11	Dichloromethane (Methylene Chloride)
12	n-Octane
13	n-Pentane
14	Perchlorethylene
15	Styrene
16	n-Propyl Acetate
17	o-Xylene
18	m-Xylene
19	p-Xylene

TABLE 2 - DATA CARD NO. 1 CONTENTS

Memory Location	Number Stored
R_0	8420779.13
R_1	5810790.30
R_2	9220867.13
R_3	4610789.33
R_4	3200791.67
R_5	8810900.22
R_6	7410714.19
R_7	10020684.11
R_8	8620660.12
R_9	6010786.20
$R_{S0}(R_{10})$	7210805.18
$R_{S1}(R_{11})$	8491327.00 *
$R_{S2}(R_{12})$	11420703.10
$R_{S3}(R_{13})$	7220626.14
$R_{S4}(R_{14})$	16581620.00 *
$R_{S5}(R_{15})$	10420906.11
$R_{S6}(R_{16})$	10210872.00 *
$R_{S7}(R_{17})$	10620880.10
$R_{S8}(R_{18})$	10620864.00 *
$R_{S9}(R_{19})$	10620861.00

* LFL data not available at time of writing.

FIGURE 1 - PROGRAM PRINTOUT

```
001  *LBL4      21 11
002   STO1      35 41
003   CF3   16 22 03
004   RTN         24
005  *LBL1      21 11
006   FS?   16 23 03
007   GTO1      22 01
008   GSB0  23 16 14
009   RCLE      36 14
010   EEX        -23
011     2         02
012     +        -24
013     ×        -35
014   RCLB      36 12
015     ×        -35
016   EEX        -23
017     2         02
018     +        -24
019   GSB5      23 05
020     +        -24
021   GSB2      23 02
022     ×        -35
023   GSB3      23 03
024     +        -24
025   RTN         24
026  *LBL0      21 14
027   FS?   16 23 03
028   GTO4      22 04
029   GSB5      23 05
030   GSB3      23 03
031     ×        -35
032   RCLC      36 13
033     ×        -35
034   GSB2      23 02
035     +        -24
036   RCLB      36 12
037     +        -24
038   EEX        -23
039     2         02
040     ×        -35
041   FIX   16 23 01
042   RTN         24
043   GSB0  23 16 14
044     +        -24
045   EEX        -23
046     2         02
047     ×        -35
048   RTN         24
049  *LBLE      21 15
050   FS?   16 23 03
051   GTO7      22 07
052   GSB5      23 05
053   EEX        -23
054     4         04
055     ×        -35
056   RCLC      36 13
057     ×        -35
058   GSB3      23 03
059     ×        -35
060   GSB2      23 02
061     +        -24
062   GSB0  23 16 14
063     +        -24
064   RCLD      36 14
065     +        -24
066   RTN         24
067  *LBL1      21 01
068   STO0      35 10
069   RTN         24
070  *LBL2      21 02
071   RCL1      36 45
072   EEX        -23
073     4         04
074     +        -24
075   INT       16 34
076     1         01
077     0         00
078     +        -24
079   RTN         24
080  *LBL3      21 03
081   RCL1      36 45
082   INT       16 34
083   EEX        -23
084     4         04
085     +        -24
086   FRC       16 44
087     1         01
088     0         00
089     ×        -35
090   RTN         24
091  *LBL4      21 04
092   STO0      35 14
093   RTN         24
094  *LBL5      21 05
095     2         02
096     4         04
097     .        -62
098     0         00
099     4         04
100     4         04
101   RTN         24
102  *LBL0  21 16 14
103   RCL1      36 45
104   FRC       16 44
105   EEX        -23
106     1         01
107     ×        -35
108   RTN         24
109  *LBL0  21 16 14
110   STO6      35 16
111   RTN         24
112  *LBL0  21 16 14
113   F0?   16 23 00
114   GTO6      22 06
115   SF0   16 21 00
116     1         01
117   RTN         24
118  *LBL8      21 08
119   CF0   16 22 00
120     0         00
121   RTN         24
122  *LBL7      21 07
123   F0?   16 23 00
124   GTO5      22 05
125   GSB3      23 03
126   STOE      35 15
127   RTN         24
128  *LBL9      21 09
129     2         02
130     3         03
131     .        -62
132     5         05
133     1         01
134     7         07
135     ×        -35
136   RTN         24
137  *LBLE      21 15
138   RCLB      36 12
139     ×        -35
140   EEX        -23
141     2         02
142     +        -24
143   RCLE      36 15
144   GSB0  23 16 14
145     ×        -35
146   EEX        -23
147     2         02
148     +        -24
149     +        -24
150   EEX        -23
151     2         02
152     ×        -35
153   GTO0      22 10
154   RTN         24
155  *LBLe      21 16 15
156   FIX   16 23 01
157   GTO6      22 06
158   SF1   16 21 01
159     1         01
160   RTN         24
161  *LBL6      21 06
162   CF1   16 22 01
163     0         00
164   RTN         24
165   R/S         51
```